



SDBS-¹³CNMR SDBS No. 1716 CDS-12-007

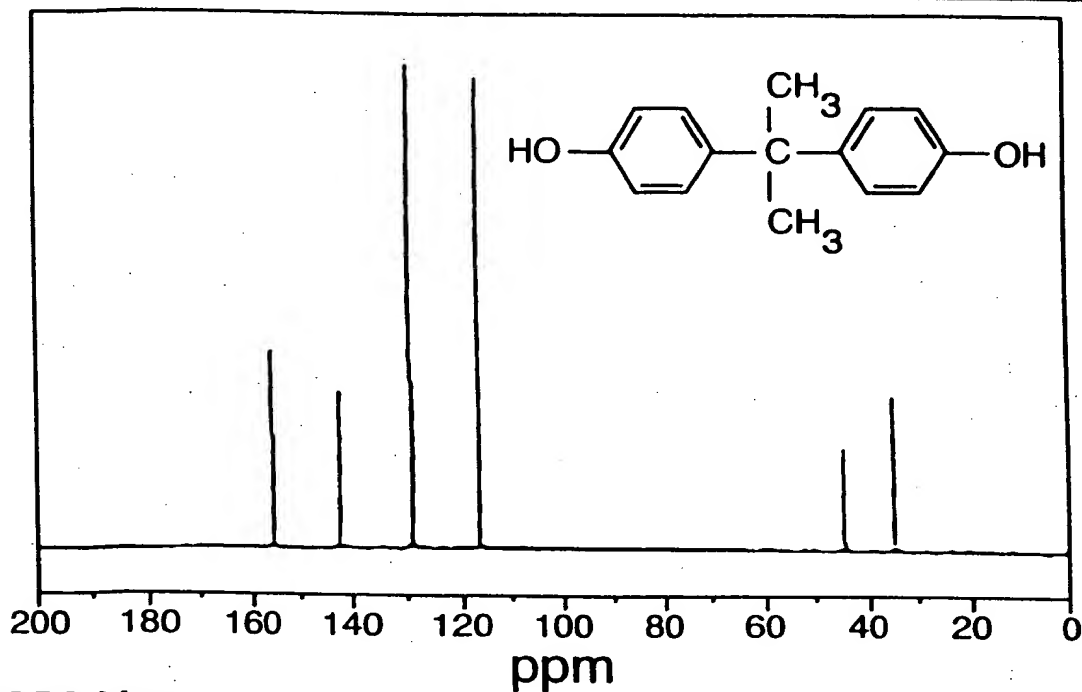
C₁₅H₁₆O₂

4, 4' - ISOPROPYLIDENEDIPHENOL

FIG. 1(a)

22.53 MHz

0.025 g : 0.5 ml DMSO-d₅



SDBS-Mass

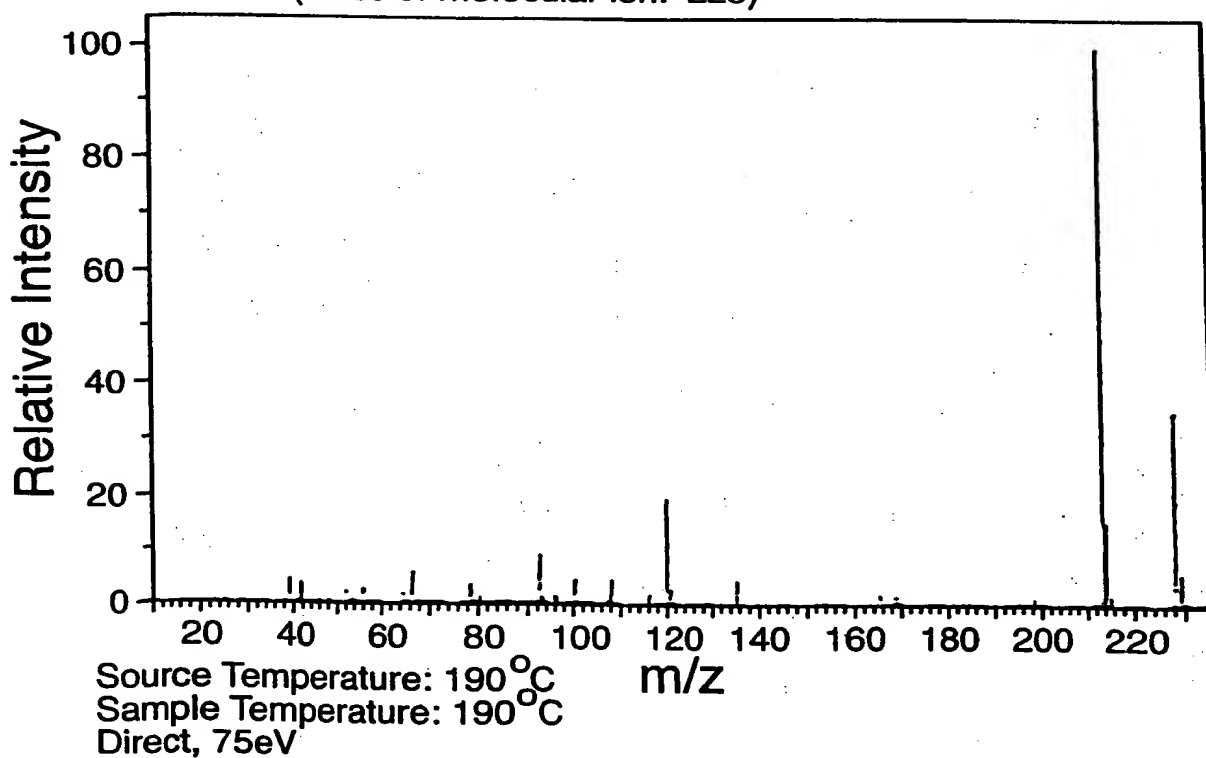
MS-NW-6834

SDBS No. - 1716

4, 4' - ISOPROPYLIDENEDIPHENOL

(Mass of molecular ion: 228)

FIG. 1(b)



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FIG. 1(c)

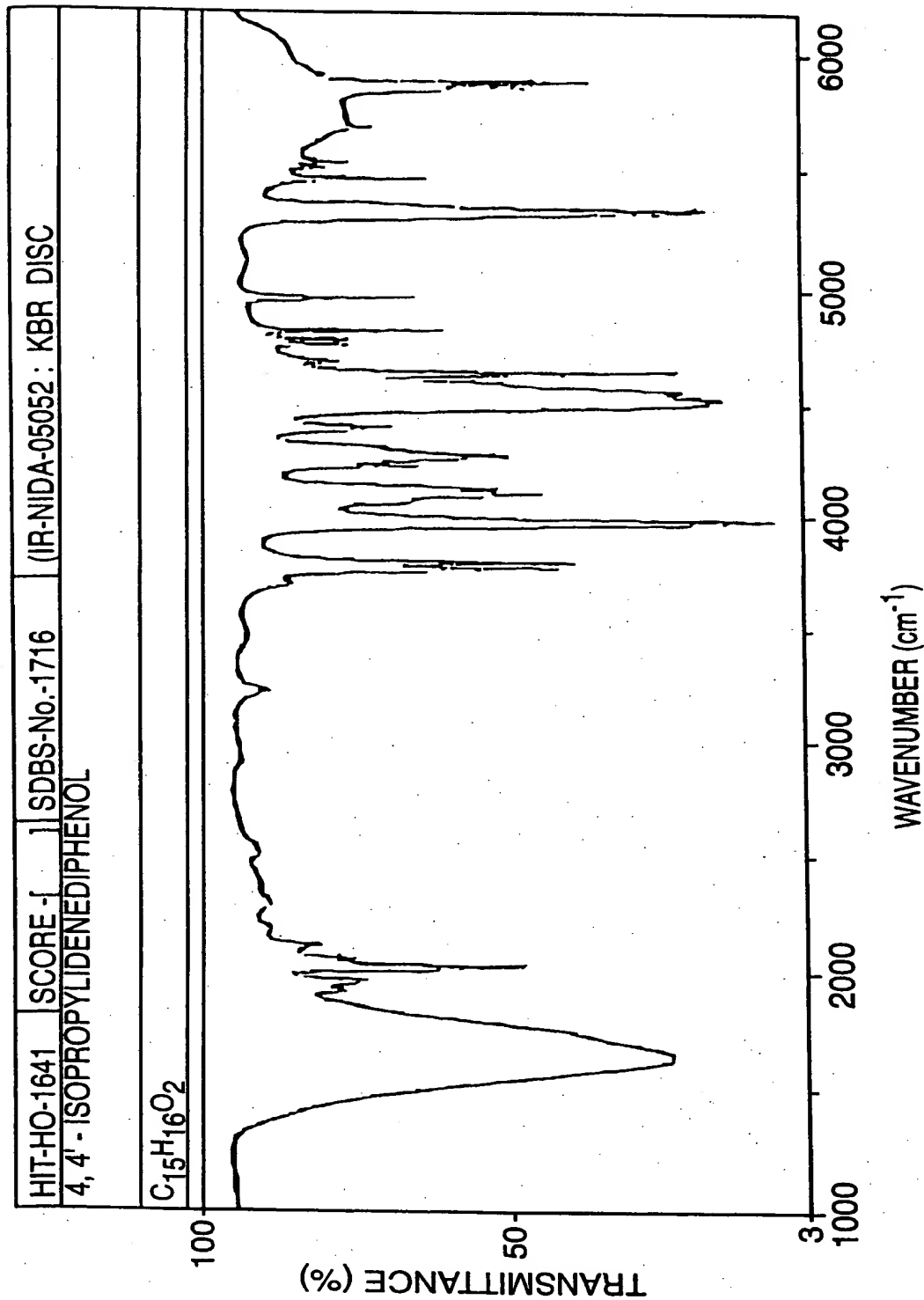
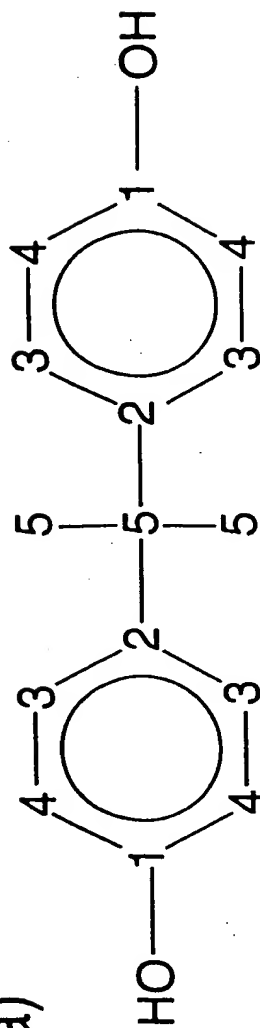


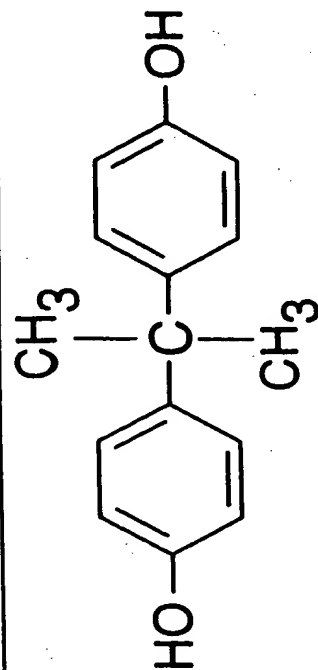
FIG. 2(a)



^{13}C	δ	ppm	Int.	Assign.
1	154.72	411		
2	140.94	330		
3	127.11	1000		
4	114.43	977		
5	40.78	223		
6	30.73	328		

FIG. 2(c)

CM^{-1}	%T	CM^{-1}	%T	CM^{-1}	%T	CM^{-1}	%T	CM^{-1}	%T	CM^{-1}	%T
3168	21	2933	72	1436	49	1178	20	816	66		
3070	74	2871	77	1384	62	1150	74	759	60		
3050	74	1512	39	1263	47	1113	72	755	77		
3030	70	1600	37	1295	66	1102	72	724	72		
2076	46	1510	4	1247	14	1085	57	650	58		
2966	45	1483	62	1239	12	1013	62	585	41		
2966	62	1447	42	1221	19	827	14	553	34		



SDBS-Mass

FIG. 2(b)

MS-NW-6834

SDBS NO. - 1716

4, 4' - ISOPROPYLIDENEDIPHENOL

$C_{15}H_{16}O_2$

/Mass of molecular ion:

228:

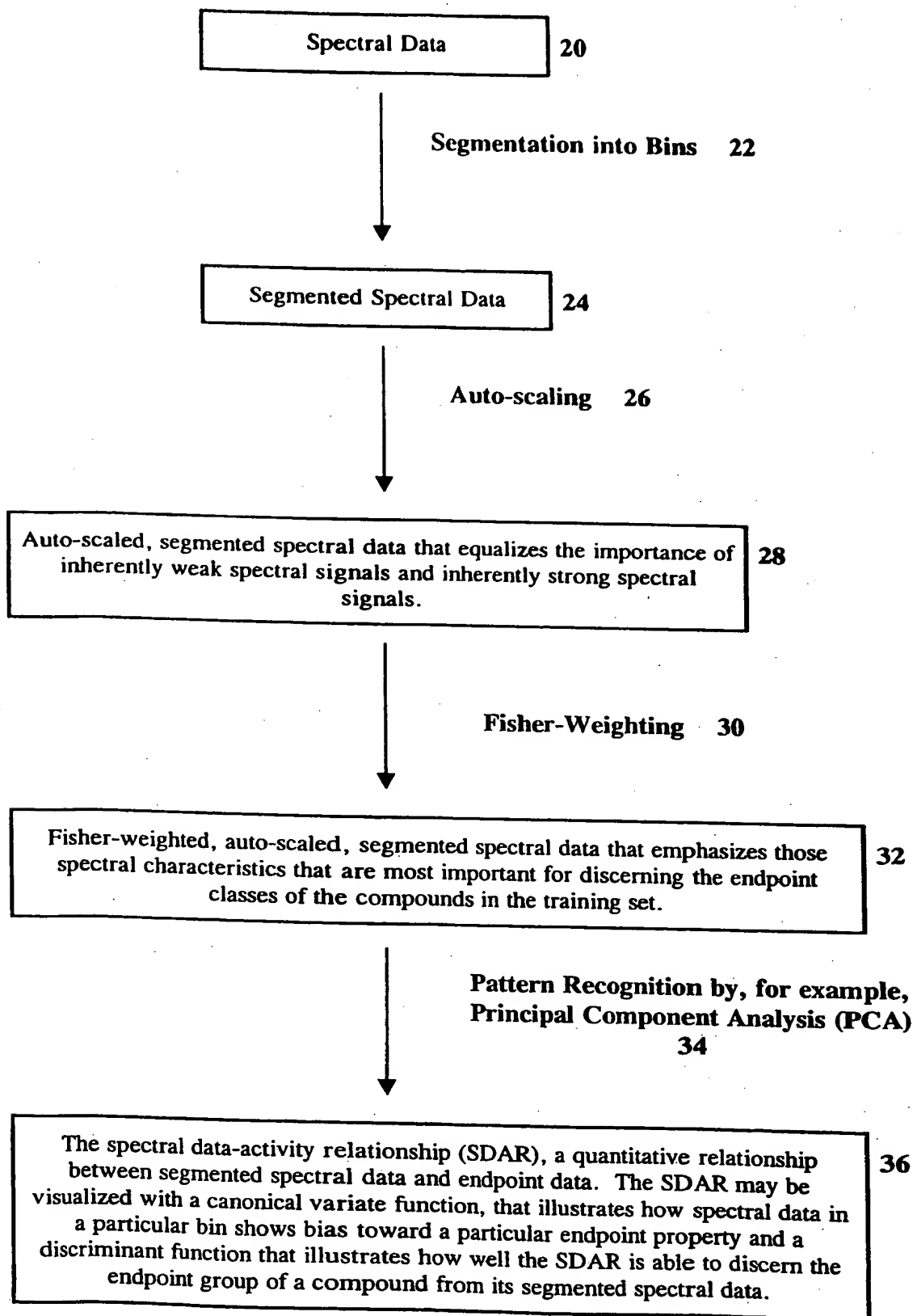
m/z ratio

27.0	1
39.0	4
41.0	3
51.0	2
55.0	2
63.0	2
65.0	5
66.0	1
76.0	1
77.0	3
79.0	1
89.0	1
90.0	1
91.0	9
92.0	1
94.0	2
95.0	1
99.0	4
105.0	1
106.5	2
107.0	4
114.0	1
115.0	1
119.0	19
120.0	2
134.0	1
135.0	4
152.0	1
165.0	2
169.0	1
181.0	1
183.0	1
195.0	1
197.0	1
198.0	1
212.0	1
213.0	100
214.0	15
215.0	1
229.0	35
239.0	5

Bin Number	Spectral Intensity	Bin Number	Spectral Intensity	Bin Number	Spectral Intensity
51	2	183	1	1025	62
55	2	195	1	1026	42
63	2	197	1	1027	49
65	5	198	1	1032	62
66	1	212	1	1034	47
76	1	213	100	1041	66
77	3	214	15	1046	14
79	1	215	1	1047	12
89	1	228	35	1048	19
90	1	229	5	1053	20
91	9	580	328	1056	74
92	1	590	223	1059	72
94	2	664	977	1060	72
95	1	677	1000	1062	57
99	4	690	330	1069	62
105	1	704	441	1088	14
106	2	834	21	1089	55
107	4	864	74	1095	60
114	1	866	74	1097	77
115	1	868	70	1098	72
119	19	873	46	1106	68
120	2	874	46	1114	41
134	1	875	62	1115	34
135	4	877	72		
152	1	883	77		
165	2	1009	39		
169	1	1011	37		
181	1	1019	4		

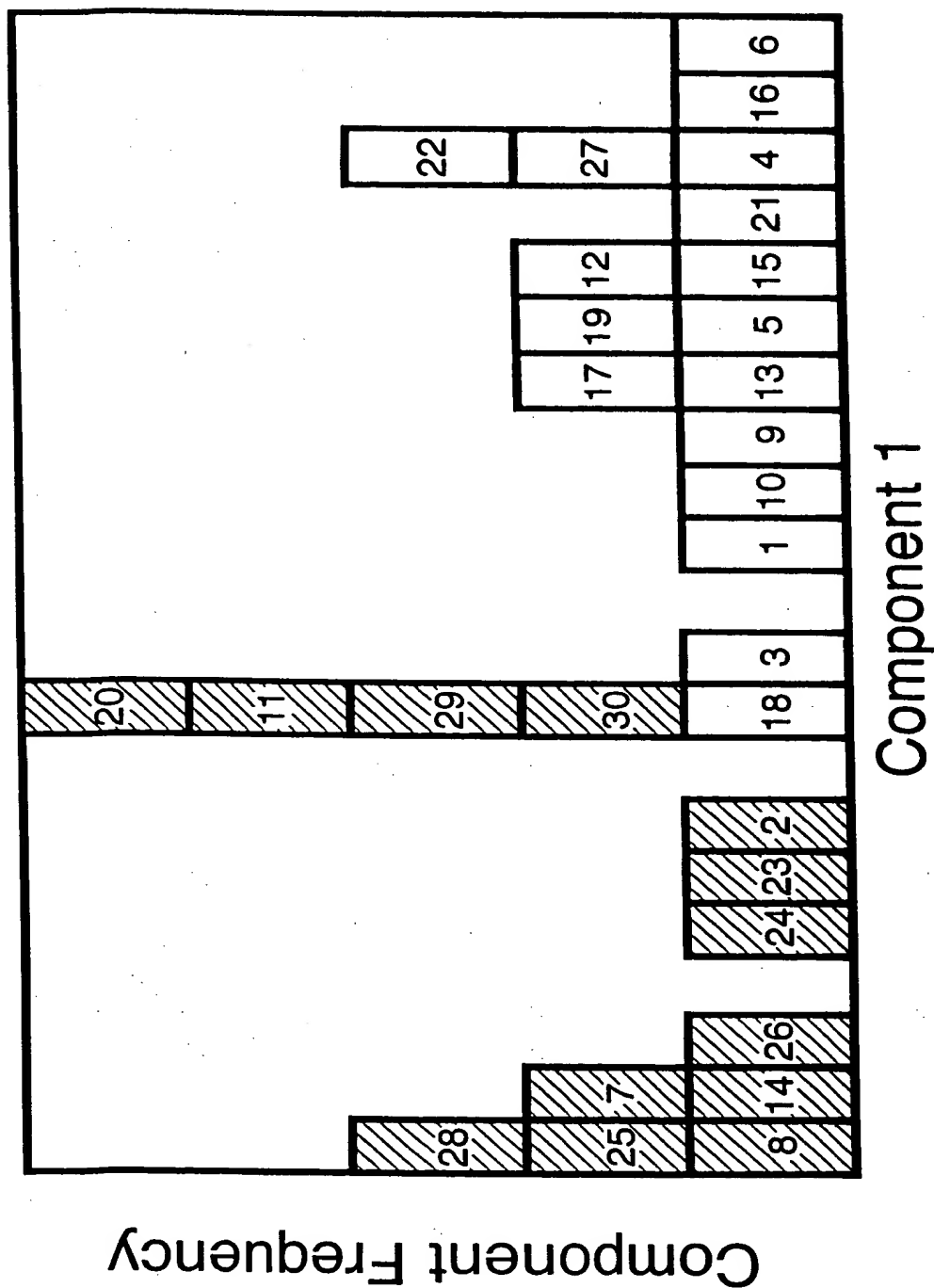
FIG. 3 – A hypothetical set of spectrally derived molecular structure descriptors for bisphenol A.

FIG. 4



DISCRIMINANT FUNCTION

FIG. 5



CANONICAL VARIATE 1

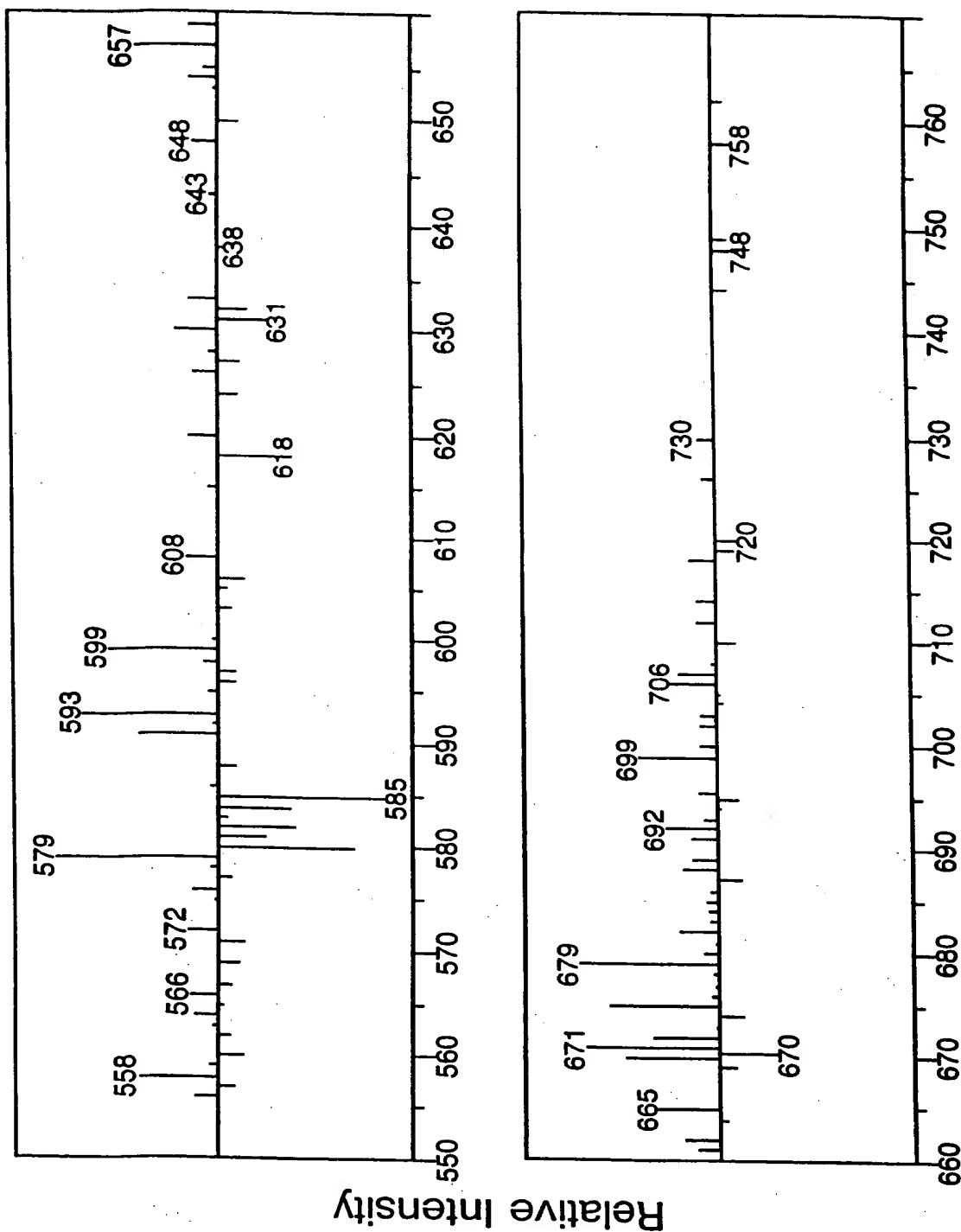
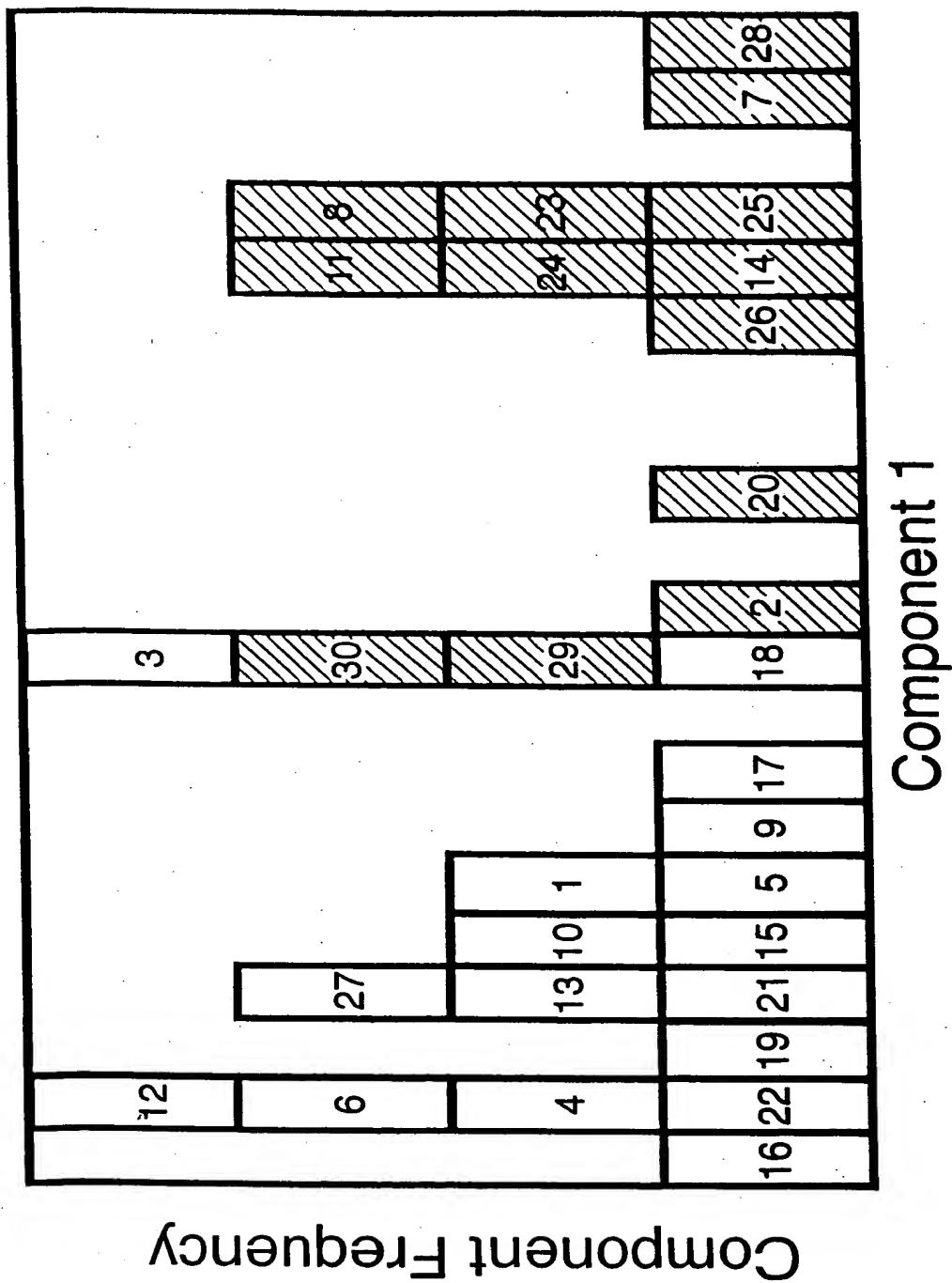


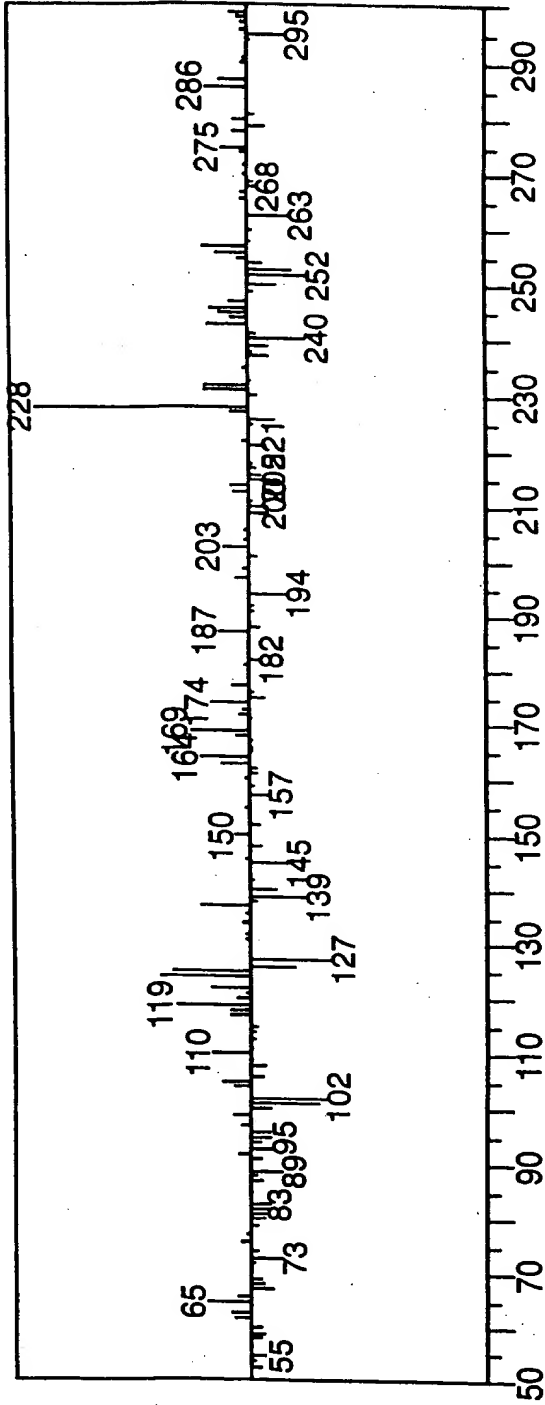
FIG. 6

M/Z

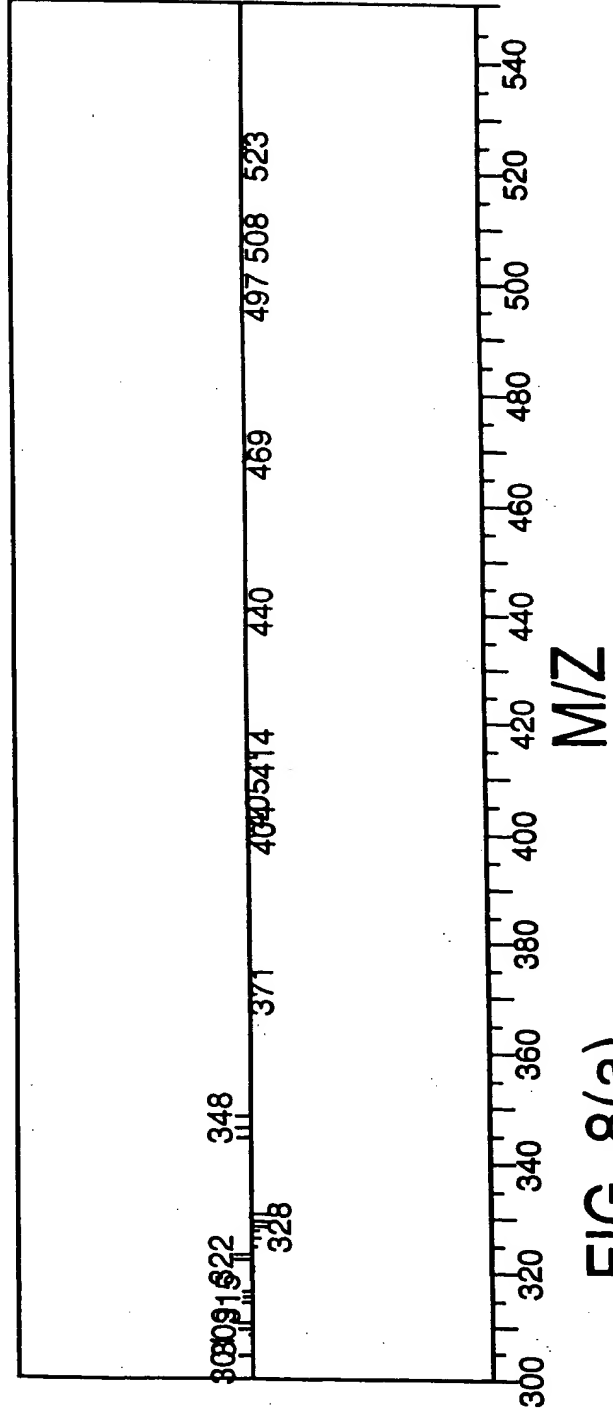
FIG. 7 DISCRIMINANT FUNCTION



CANONICAL VARIATE 1



Relative Intensity



M/Z

FIG. 8(a)

CANONICAL VARIATE 1

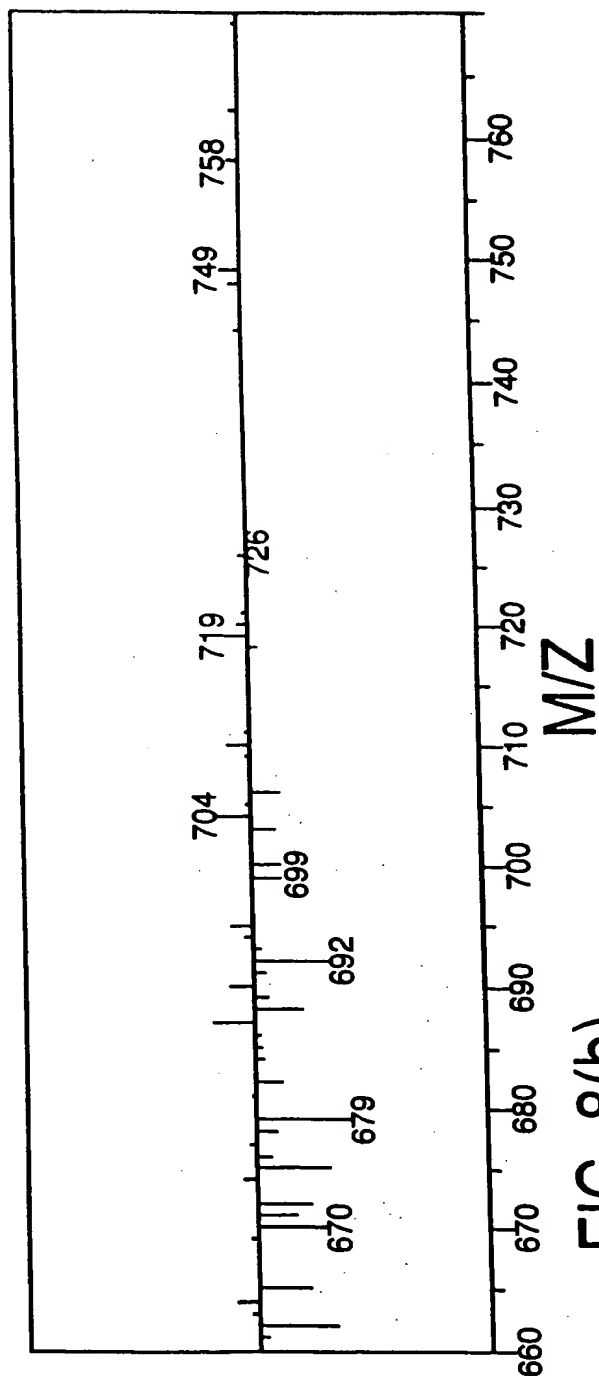
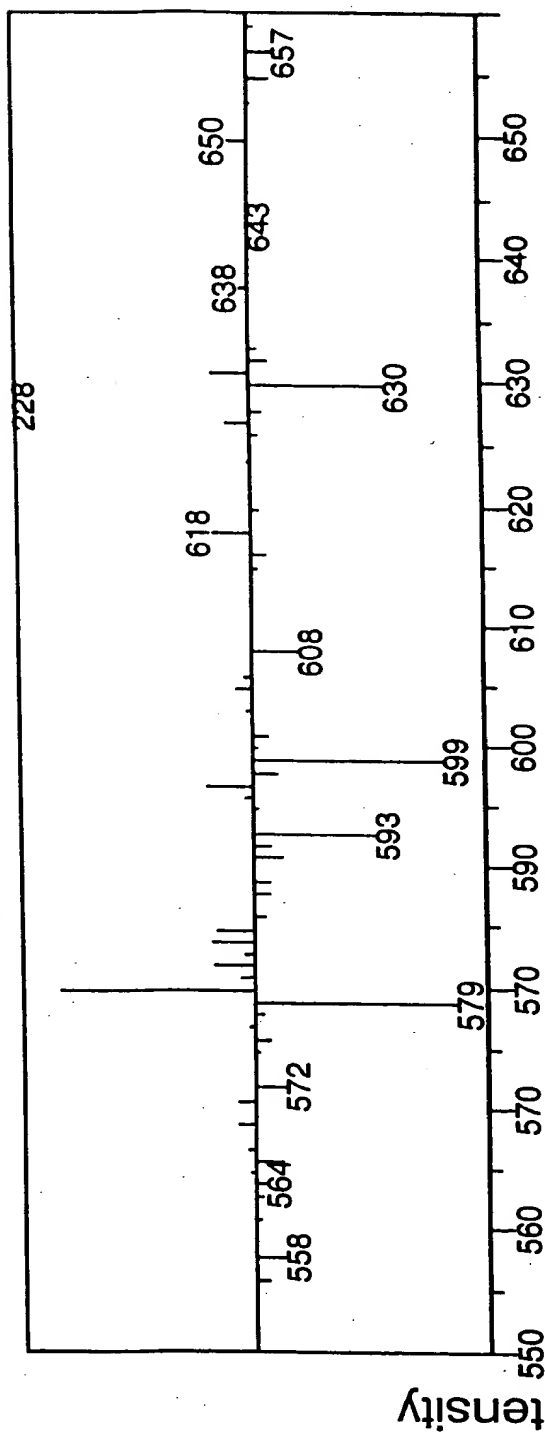


FIG. 8(b)

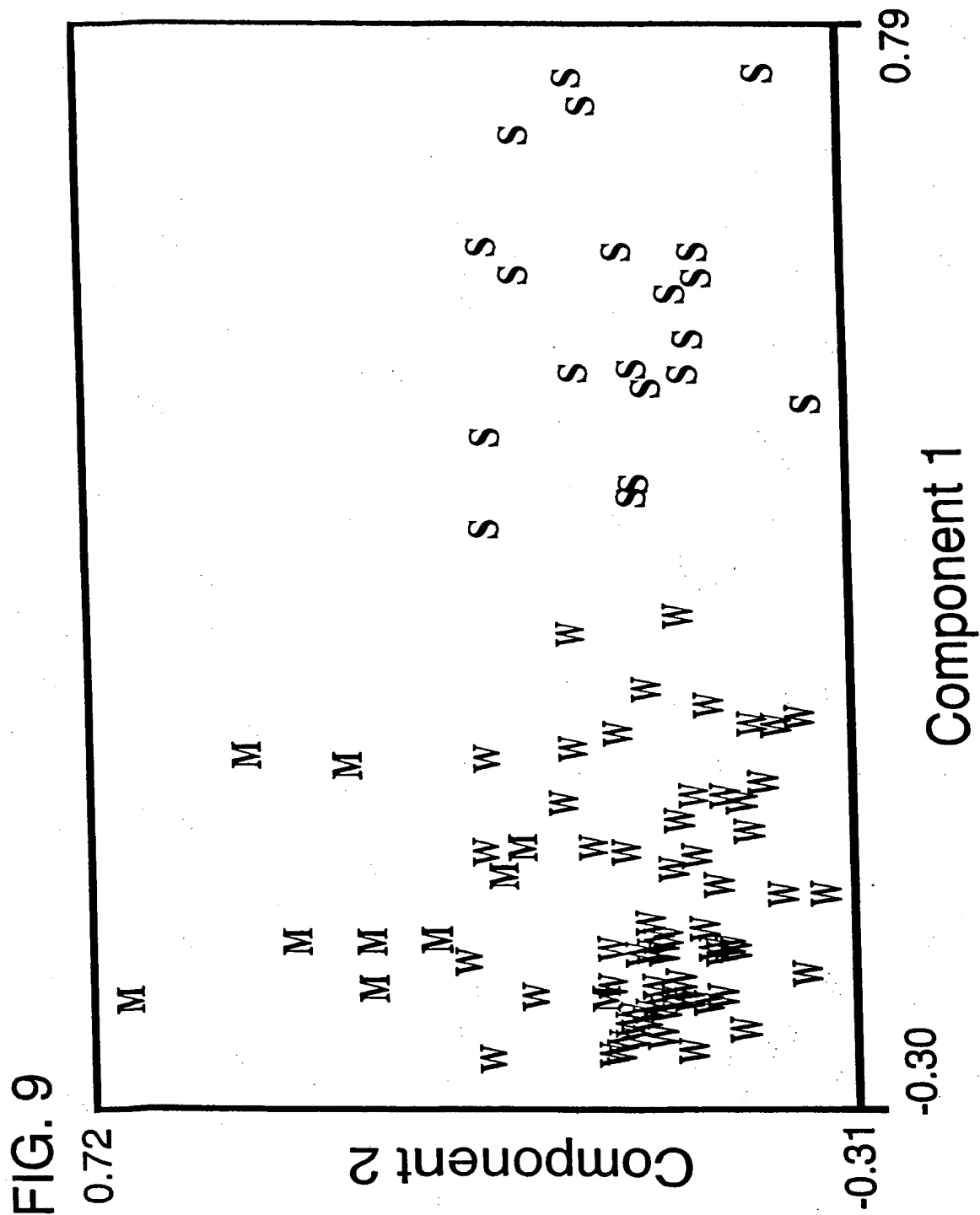


FIG. 10

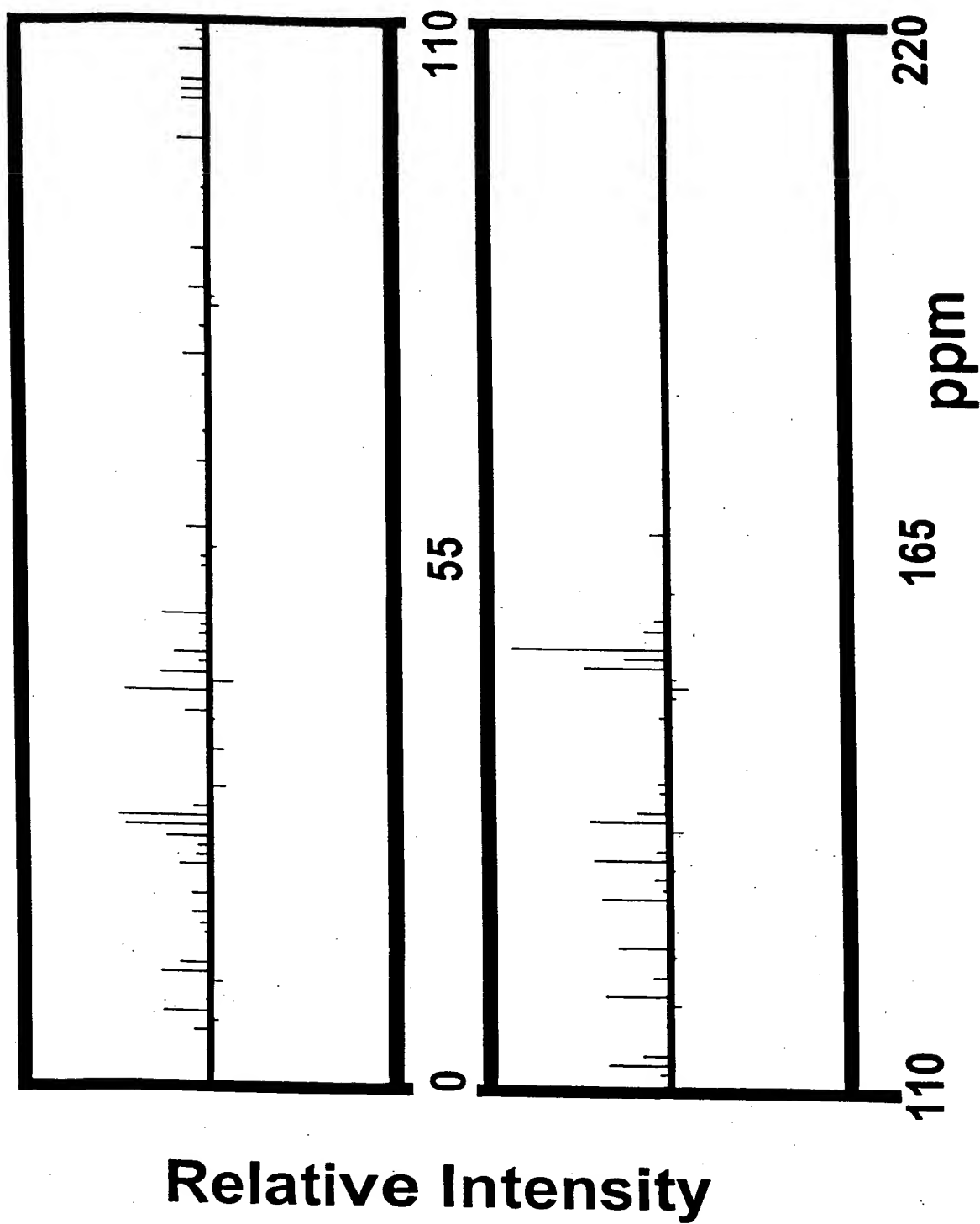


FIG. 11

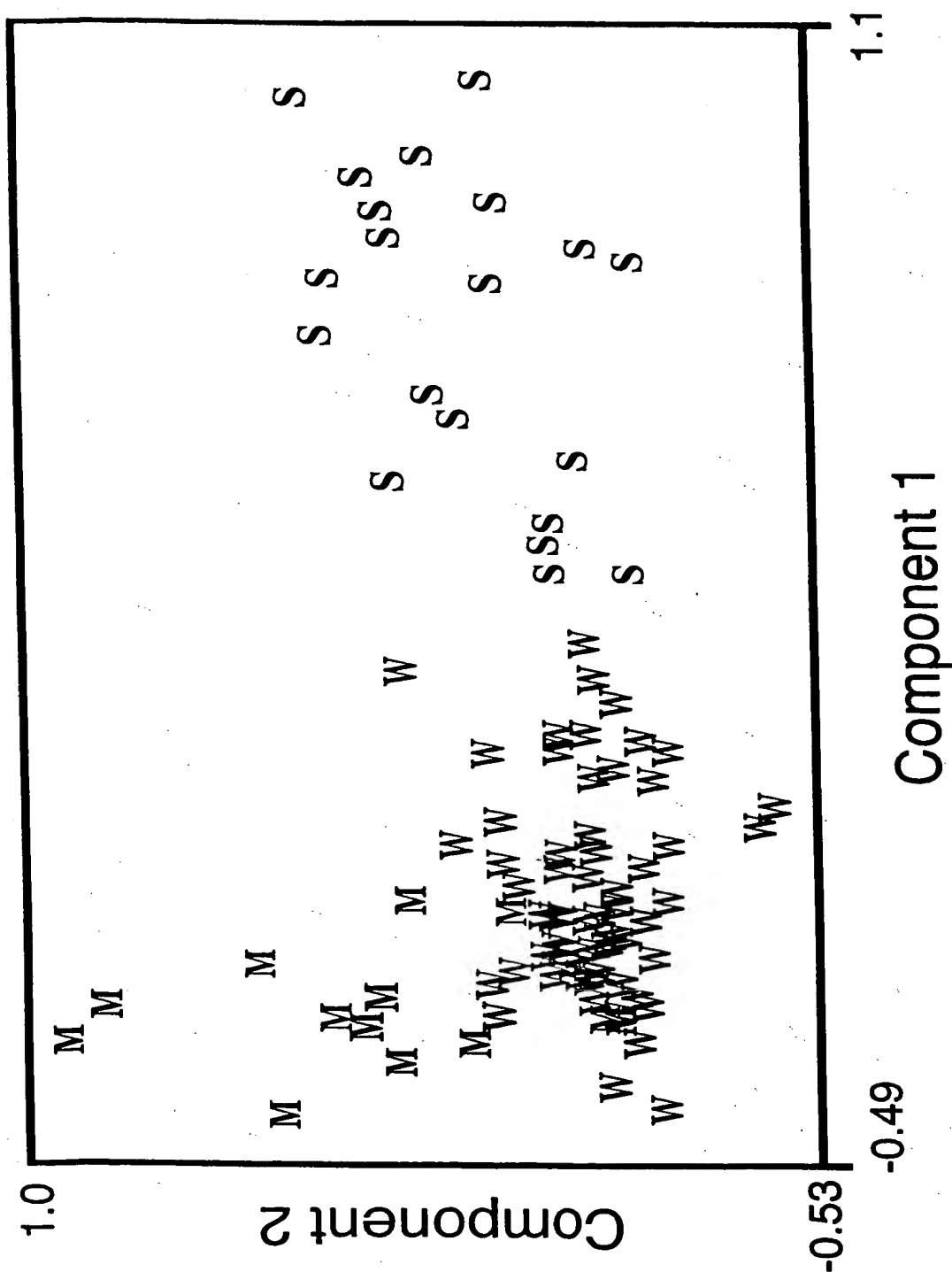


FIG. 12(a)

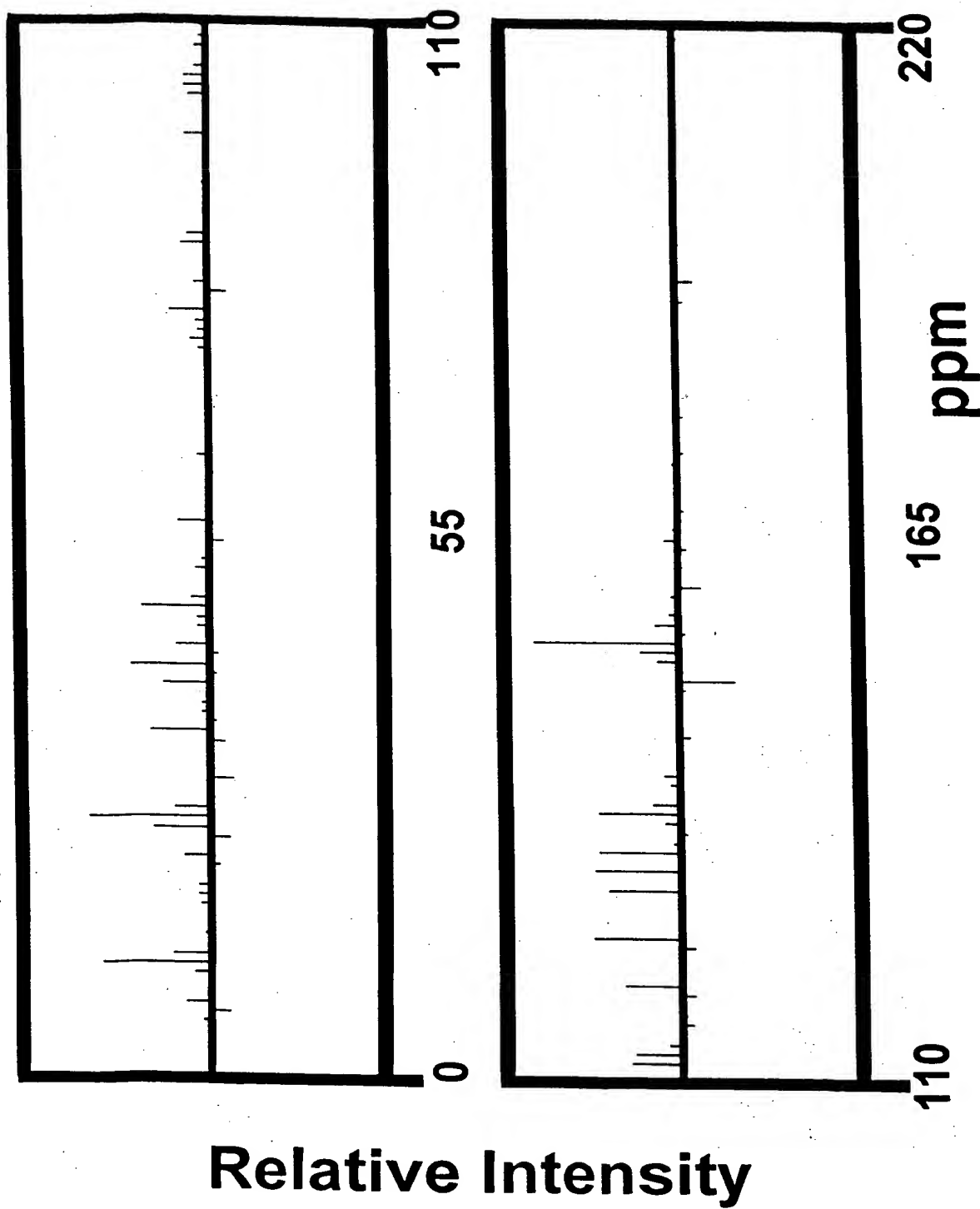
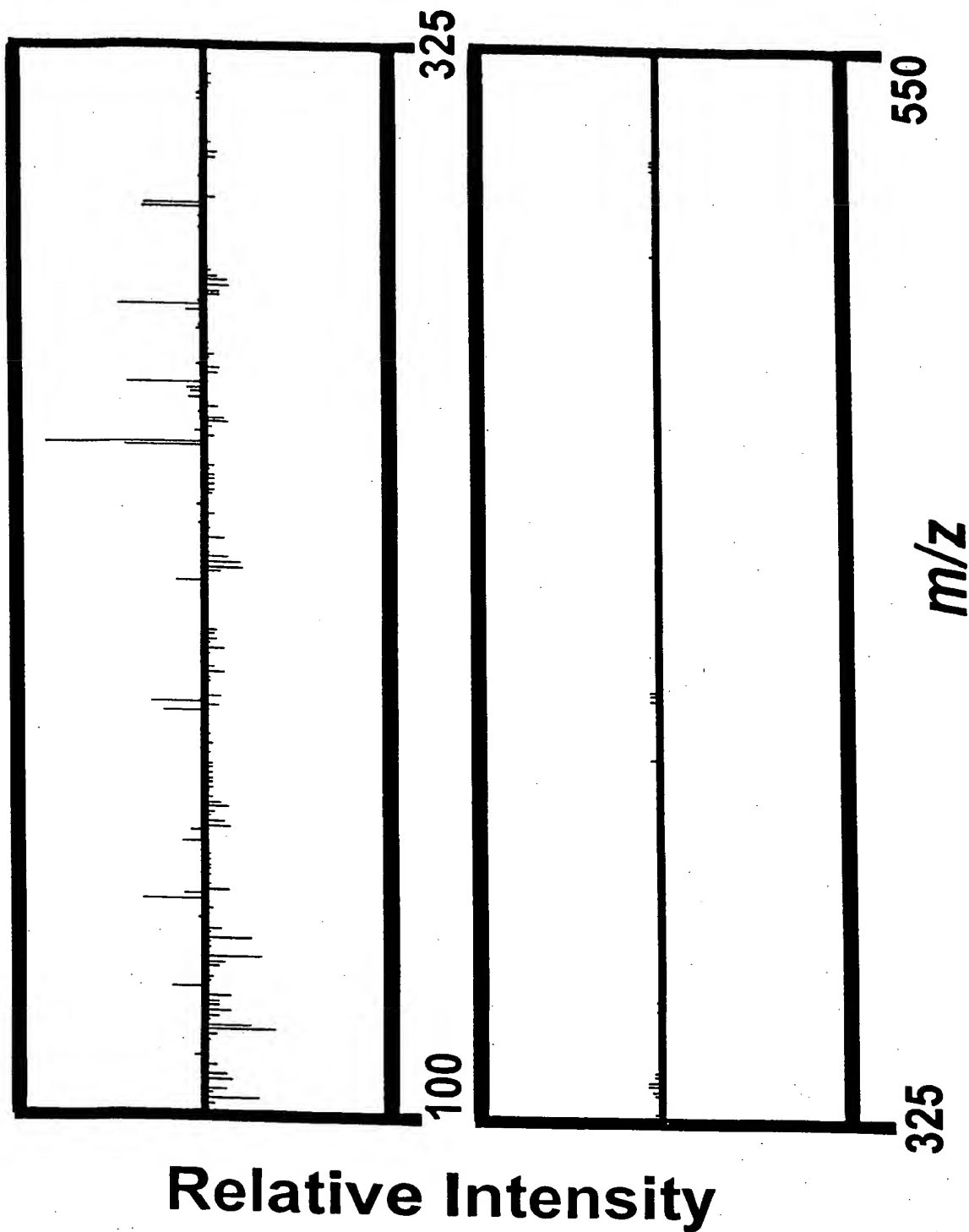


FIG. 12(b)



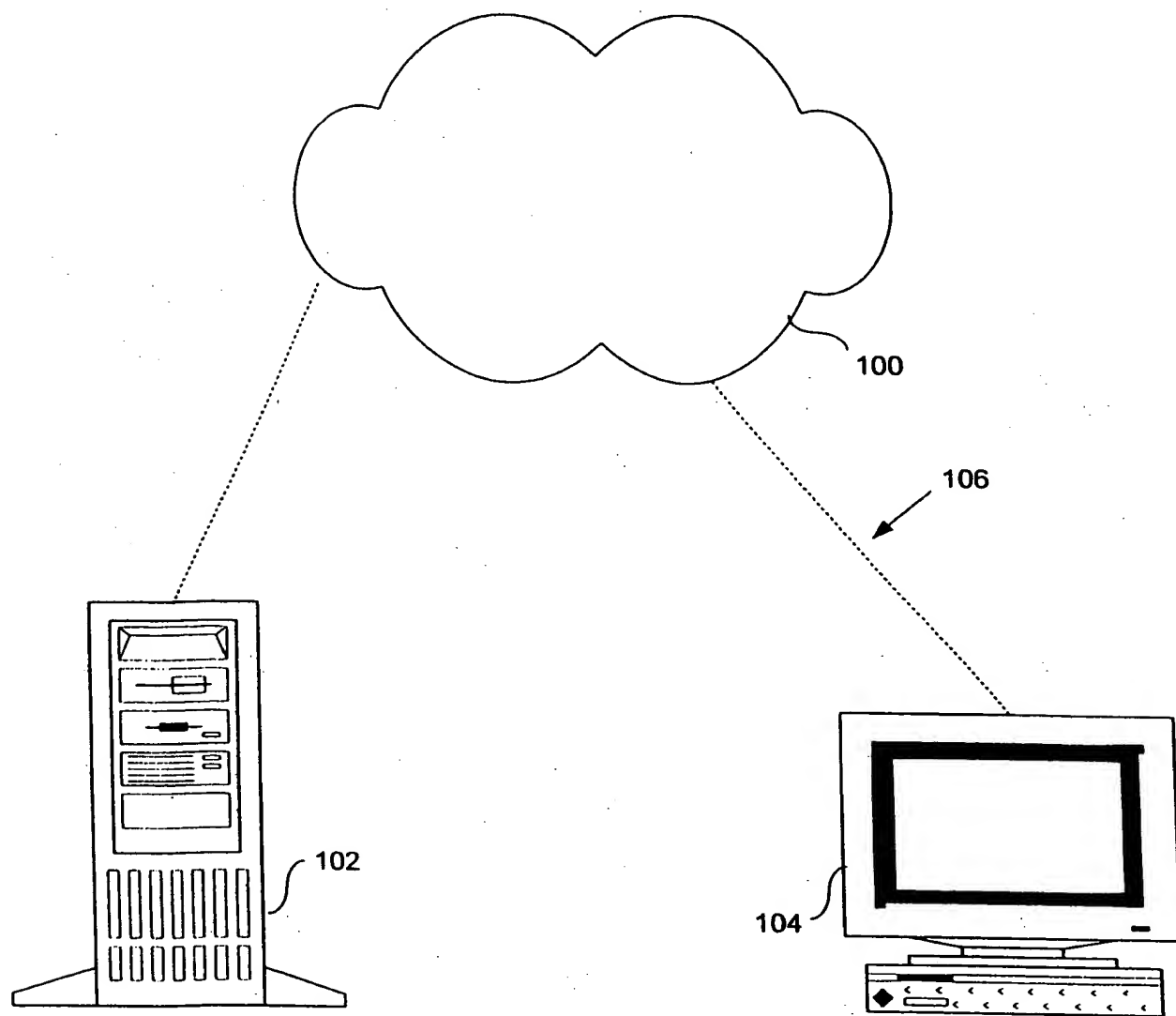
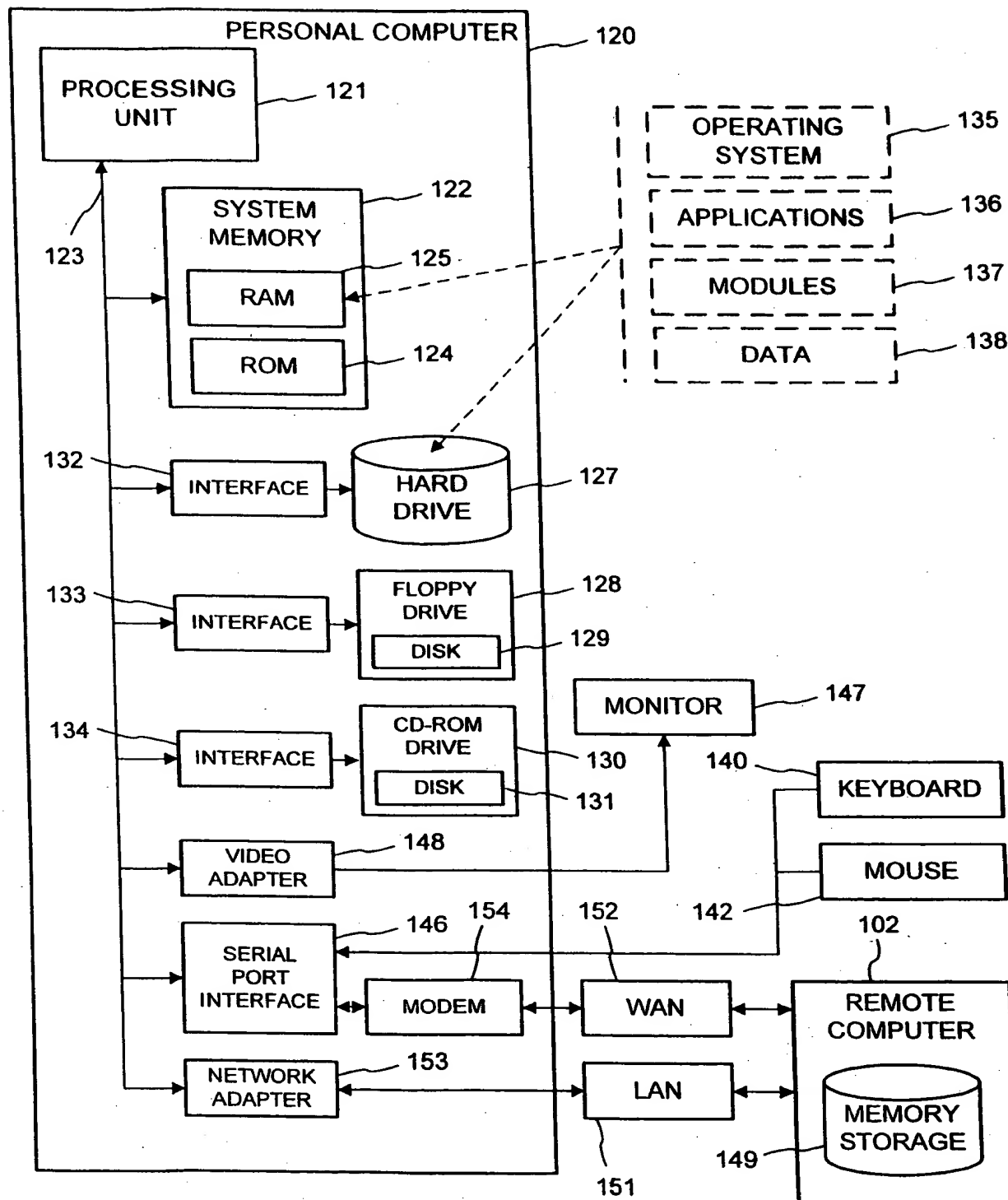


FIG. 13

FIG. 14



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